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臭牡丹中一个新的过氧化物*

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摘要：从四川眉山地区产的臭牡丹（*Clerodendrum bungei* Steud.）地上部分分离到一个新的过氧化物，命名为 bungein A. **其结构通过各项波谱分析得到鉴定，这是首次从马鞭草科鄣桐属植物中分到的过氧化物。**

关键词：马鞭草科；臭牡丹；过氧化物；bungein A
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A New Peroxide Compound from *Clerodendrum bungei* *

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Abstract：A new peroxide compound，bungein A，was isolated from the aerial parts of *Clerodendrum bungei* Steud. collected at Meishan County，Sichuan，China. Its structure was elucidated by the spectroscopic methods. The peroxide compound was obtained from *Clerodendrum* genus for the first time.

Key words：*Clerodendrum bungei*；Verbenaceae；Peroxide compound；Bungein A

Clerodendrum bungei Steud.，a shrub in the Verbenaceae family，distributed widely in most provinces of China. It has been used as folk medicine to treat headache，dizziness，furuncle（Wu *et al*，1977）and hysteroptosis（Zhou *et al*，1982）for a long time. Up to now，only a few papers（Zhou *et al*，1982；He *et al*，1997）concerned the chemical study of this plant. In order to find its biologically active components，this medicinal plant was reinvestigated carefully.

The study on *Clerodendrum bungei* led to the isolation and characterization of a new peroxide compound，bungein A.

Bungein A（**1**），no optical rotation，was obtained as colorless wax. Its molecular formula（$C_{16}H_{18}O_4$）was deduced from EIMS spectrum（m/z 274 $[M]^+$）and ^{13}C NMR spectrum. The IR absorption bands pointed to the presence of free hydroxyl groups（3147－3391 cm^{-1}）and aromatic rings（1599，1512 and 819 cm^{-1}）. The UV spectrum of **1** showed absorption maxims at 224，278.5 and 281.5 nm，

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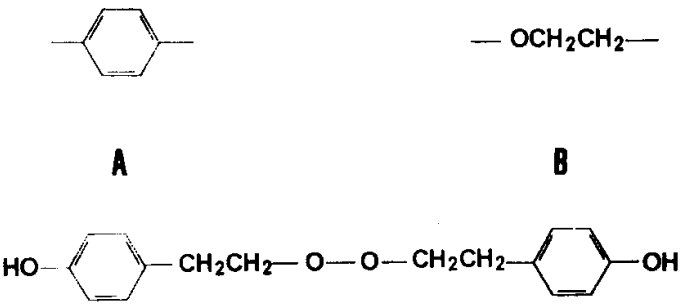
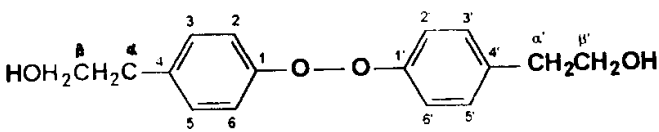
which also suggested the existence of benzene moieties. Its ^{13}C NMR (Table 1) spectrum revealed only six carbon signals in **1**: two quaternary carbons (156.5 and 130.8 ppm), two methines (δ130.7 and 115.8 ppm), and two methylenes (δ64.2 and 39.3 ppm), exhibiting that **1** was a symmetric molecular. Its ^{1}H NMR (Table 1) spectrum displayed four groups of proton signals: δ7.03 (4H, dd, J = 8.4 and 2.9 Hz) and 6.73 (4H, dd, J = 8.4 and 2.9 Hz) due to aromatic protons, δ3.69 (4H, t, J = 7.2 Hz) owing to two equivalent methylenes bearing oxygen and 2.70 (4H, t, J = 7.2 Hz) assigned to two equivalent methylenes. Analysis of the coupling pattern of protons indicated the presence of some partial structures such as **A** and **B** (Fig. 1). From the above discussion, two possible structures **C** and **1** (Fig. 1) were suggested. In addition, **1** gave positive reaction with the reagent of Farbentwickler 3 merk; and after reacting with triphenyl phosphine, the above reaction was negative. It indicated 1 was a peroxide compound (Lou *et al*, 1997). This conclusion was also supported by the downfield carbon signals δ156.5 ppm (C－1 and C－1).





1

Table 1　The ^{1}H and ^{13}C NMR spectral data of compound **1** in CD_3COCD_3 (400 MHz and 100.6 MHz, δ from TMS, J in Hz)

H/C	δ_H	δ_C
1, 1′		156.5 (s)
2, 6, 2′, 6′	6.73 (4H, dd, J=8.4, 2.9)	115.8 (d)
3, 5, 3′, 5′	7.03 (4H, dd, J=8.4, 2.9)	130.7 (d)
4, 4′		130.8 (s)
α, α′	2.70 (4H, t, J=7.2)	39.34 (t)
β, β′	3.69 (4H, t, J=7.2)	64.21 (t)

Moreover, further examination of the EIMS spectrum (m/z 274 $[M]^+$ (27), 256 $[M-H_2O]^+$ (4.5), 243 $[M-CH_2OH]^+$ (45), 225 $[256-CH_2OH \text{ or } 243-H_2O]^+$ (23) and 138 (19)) of **1** excluded the structure **C**, since it can not explain the fragmentation pattern of EIMS of **1**. Accordingly, bungein A was identified as **1**. The structure of **1** containing a symmetric center and surface was consistent with no optical rotaion.

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